Comparison of advanced numerical models for multiphase modelling: Baer-Nunziato and Godunov-Peshkov-Romensky approaches

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Abstract

This paper represents an overview of the most promising numerical methods for multiphase modelling and its comparison on the example of known multiphase problems. Namely we will discuss Baer-Nunziato(BN) and recently proposed Godunov-Romosky-Peshkov(GPR) approaches. A distinctive and very important property of these approaches is its hyperbolicity that provides a well-posedeness of the problem. In turn, it allows to apply well-developed numerical schemes. We will see that this property is achieved by the methods described by different ways, employing different ideas of formulation of governing equations. A complementary conservation equation is used in BN model, while GPR model takes an idea of applying of a distortion tensor to build a governing system of equations. It makes possible to obtain a unified mathematical model both for fluids and solids problem in frame of GPR model. That fact opens a very wide range of its application.

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Introduction

Multiphase flows are the omnipresent phenomena in our life. From particle interactions in molecular clusters up to behavior of star nebulas, in a number of scientific and engineering disciplines. Ground processes in geology, airflows in aerospace tasks, reactive media in chemistry and biology, different scales of problems in astronomy – are just several examples of multiphase presence. A development of computational simulation of these problems, as an efficient tool to study different sides of the problem where a physical experiment can be intricate or not possible, is on behalf of many analytical and industrial research.

Among all the methods proposed for the multiphase flows modelling one can pick out two remarkable ones that describe the flow via the *hyperbolic* system of equations. These are proposed by Baer and Nunziato model ([1], further denonted as BN) and model by Godunov and Romenski ([2]), recently advanced to the unified hyperbolic formulation of fluid and solid dynamics, in [3, 4] (further denoted as GPR model).

Hyperbolicity of the system supplies the well-posedness of the problem, that is extremely important for mathematical modelling ([5]).

In frame of BN model additional conservation relations are introduced to close the system and it gave quite accurate results for mixture, allowed to capture an interface in multiphase problems. BN model gives a hyperbolic system but not all of the equations are in conservative form, it put some difficulties in the definition of the discontinuous solution and in the development of very high order numerical methods.

GPR model presents both features- hyperbolicity and a conservative form of all the equations of the system. These two specialties provide very good mathematical properties including continuous dependence of the solution on the initial data and the finite velocity for perturbation propagation. That makes model advantageous as it allows to apply known accurate numerical methods (like recent ADER scheme for example, [6, 7]).

This paper represents a comparison between well-established BN and new GPR model approaches. In the sections below there are a brief description of both methods and comparison of numerical experiments performed after these methods, a conclusion is given in the last part.

Brief description of hyperbolic models

Baer-Nunziato approach

Several approaches were developed for numerical simulation of systems containing several different phases. Some systems of governing equations were constructed using an averaging of flow variables [8], using continuum mixture theory [9] and etc. In general all they revealed a closure problem for system of equation, as a supplementary independent kinematic variable (as volume fraction for example) is included.

To bypass that obstacle some additional conditions were applied, like relation for pressure equilibrium between the phases, or a definition pressure in the solid phase in terms of the configuration changes of the granular material (particularly for detonation problems). That imposed some constraints to the range of applicability of the methods. Substantially the difficulty of modelling was stuck on the issue of describing a compressibility of each phase and compaction of the solid phase.

BN approach accounts for these effects using an additional conservation equation for the volume fraction of the solid with the help of evolutionary equation for the volume fraction consistent with thermodynamics. It was firstly shown for the numerical simulation of the two phase reactive flows where a perturbation passed through the mixture of gas and small solid particles in frame of the deflagration or detonation processes([1]). The governing equations are the composition of two separate systems of the conservation laws for each phase, coupled by interface exchange terms ([10]).

Thus obtained system of equations became hyperbolic. But not all the equations have a conservative form. For two phase flow system reads:

$$\begin{aligned}
\frac{\partial \alpha_m}{\partial t} + V_i \frac{\partial \alpha_m}{\partial x} &= \mu (P_{m1} - P_{m2}) \\
\frac{\partial \alpha_m \rho_m}{\partial t} + \frac{\partial \alpha_m \rho_m u_m}{\partial x} &= 0 \\
\frac{\partial \alpha_m \rho_m u_m}{\partial t} + \frac{\partial \alpha_m \rho_m u_m^2 + \alpha_m P_m}{\partial x} &= \delta_m \left[P_i \frac{\partial \alpha_m}{\partial x} + \lambda (u_{m2} - u_{m1}) \right] \\
\frac{\partial \alpha_m \rho_m E_m}{\partial t} + \frac{\partial u_m (\alpha_m \rho_m E_m + \alpha_m P_m)}{\partial x} &= \delta_m \left[P_i V_i \frac{\partial \alpha_m}{\partial x} + \mu P_i (P_{m1} - P_{m2}) + \lambda V_i (u_{m2} - u_{m1}) \right]
\end{aligned} \tag{1}$$

Here index $m = 1, 2$ - corresponds to phase 1 and 2 ($m1$ and $m2$ - when there is a difference between parameters of each phase), δ_m is equal to '1' for the first and '-1' for the second phase. α, ρ, u - are the volume fraction, density and velocity of each phase. μ and λ - are the relaxation parameters conformed to dynamic compaction viscosity and drag force (for pressure and velocity relaxation respectively). They are finite within two-phase flow regions and while instanteneous relaxation, and infinite at the interface. P_i, V_i - pressure and velocity at the interface.

GPR approach

GPR model takes an idea of continuum particles (or material elements) of small finite scale as a means to describe a changing of the media. These continuum particles represent deformable ensembles of molecules existing during a finite time and rearrangements of which actually defines a flow phenomenon, [4]. Elastic stretching of microscopic bonds between

continuum particles results in internal resistance to flow (i.e. viscosity). The time of rearrangement embodies a fluidity of a media. An admissible length scale and rearrangement time were proposed in [4, 11]. Roughly saying, a large time values maps a solid material, time value tending to zero maps an ideal gas.

Mathematical analysis [5] leads to a first order hyperbolic system of equations where viscous stresses are computed from the so-called distortion tensor $\mathbf{A}$. That tensor $\mathbf{A}$ reflects a deformation of particles and is one of the primary state variables. A stiff source term in governing system accounts for strain relaxation in the evolution equations of $\mathbf{A}$ and rearrangement time τ.

Rearrangement time τ can be taken as constant for the Newtonian flows while the dependence of τ on tensor $\mathbf{A}$ reflects the non-Newtonian properties of fluids transition from elastic to plastic regime in solids.
The system of governing equations reads:

$$\begin{aligned}
&\frac{\partial \alpha_{m1}}{\partial t} + U\frac{\partial \alpha_{m1}}{\partial x} = -\frac{\lambda_{grp}}{\rho}(P_{m2} - P_{m1}) \\
&\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \\
&\frac{\partial \rho u_m}{\partial t} + \frac{\partial (\rho u_m u_i + p\delta_{mi} - \sigma_{mk})}{\partial x_i} = 0 \\
&\frac{\partial A_{mk}}{\partial t} + \frac{\partial A_{mi} u_i)}{\partial x_i} + u_i\left(\frac{\partial A_{mk}}{\partial x_i} - \frac{\partial A_{mi}}{\partial x_k}\right) = -\frac{\psi_{km}}{\theta(\tau)} \\
&\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E u_i + (p\delta_{mi} - \sigma_{mi}))}{\partial x_i} = 0
\end{aligned} \tag{2}$$

Where ρ, u, p, E, σ retain their usual meaning of density, velocity, pressure, energy and stress tensor respectively. $\mathbf{A}$ - distortion tensor, source term $\psi_{km} = \frac{\partial E}{\partial A_{km}}$. $\theta(\tau)$ - positive scalar function corresponding to the properties of studied material, that will be specified below.

An important role in the system plays an energy definition. It is suggested to be composed of three scale components. Microscale of medium's molecules that depends on the local density and entropy (internal energy); mesoscale corresponding to the scale of material element (ensemble of molecules) - this one depends on the distortion tensor, and macroscale component for the flow scale (conventional kinetic energy).

Equation of state employed in this work are as follows:
- Internal energy (microscale part) $E_1(\rho, s)$

$$E_1(\rho, s) = \frac{c_0^2}{\gamma(\gamma-1)}\left(\frac{\rho}{\rho_0}\right)^{\gamma-1} e^{S/c_v} + \varsigma\frac{\rho_0 c_0^2 - \gamma p_0}{\gamma\rho}$$

where $\varsigma = 0$ in case of ideal gas, and $\varsigma = 1$ in case of stiffened gas or liquid.
indexes '0' correspond to some reference values

- Mesoscale part $E_2(A)$

$$E_2(s) = \frac{c_s^2}{4} dev(\mathbf{G}) dev(\mathbf{G})$$

with dev($\mathbf{G}$) - trace-free part of the tensor $dev(\mathbf{G}) = \mathbf{A}^T\mathbf{A}$.

The c_s is the characteristic velocity of propagation of transverse perturbations. It may be laid as a constant approximate value or calculated from the value of phase velocity $V(\omega)$ corresponding to disappearance of dispersion, $V(\omega) = \sqrt{c_0^2 + 4/3c_s^2}$ (an effect called as well as 'high frequency limit'). More detailed description can be found in [4, 3].
- Macroscale part, specific kinetic energy per unit mass $E_3(u)$

$$E_3(u) = \frac{1}{2} u_i u_i$$

The definition of c_s noted above is important as well for estimation of relaxation time τ, standing in the right part of PDEs. The fact of the mater that relaxation time, or time of rearrangement of material elements, is a mark of the fluidity behaviour of the medium, hence a relation between time τ and the viscosity coefficient η takes place: $\eta = \frac{\rho_0}{6}\tau c_s^2$ (see details in [3], section 3.1).

Thus, deformable material elements with the 'life time' (time before rearrangement) defining a fluidity of the medium permit to introduce a distortion tensor, that in its turn, gives a way to treat viscous fluids as generalized visco-plastic solids. This is a key aspect of GPR model.

Numerical experiments

We show in this section the results of GPR numerical solution of the one-dimensional shock-tube test with two fluids and its comparison with the results obtained in frame of BN model ([12]).

The computational domain represents a shock tube filled on the left side with high-pressure liquid water and with air at normal conditions on the right side. Initial data are as follows:
Left side: (water) ρ=1000kg/m^3, $p = 10^9 Pa$, u=0 m/s, γ=4.4.
Right side: (air) ρ=50kg/m^3, $p = 10^5 Pa$, u=0 m/s, γ=1.4.
A regular mesh with 1002 cells is used.
The time step size is calculated via CFL number, which is kept with a value 1e-2 at the first 10 steps of the calculation and than 0.9 for the rest.

The master system (2) should be complemented with closure relations. For that purpose an equation of state is defined in the form of the generalized internal energy E as a function of parameters of state, described in a section above. Then pressure of each phase is computed

as a function of total energy derivative ad is as follows: :

$$p = \rho^2 \frac{\partial E}{\partial \rho}$$

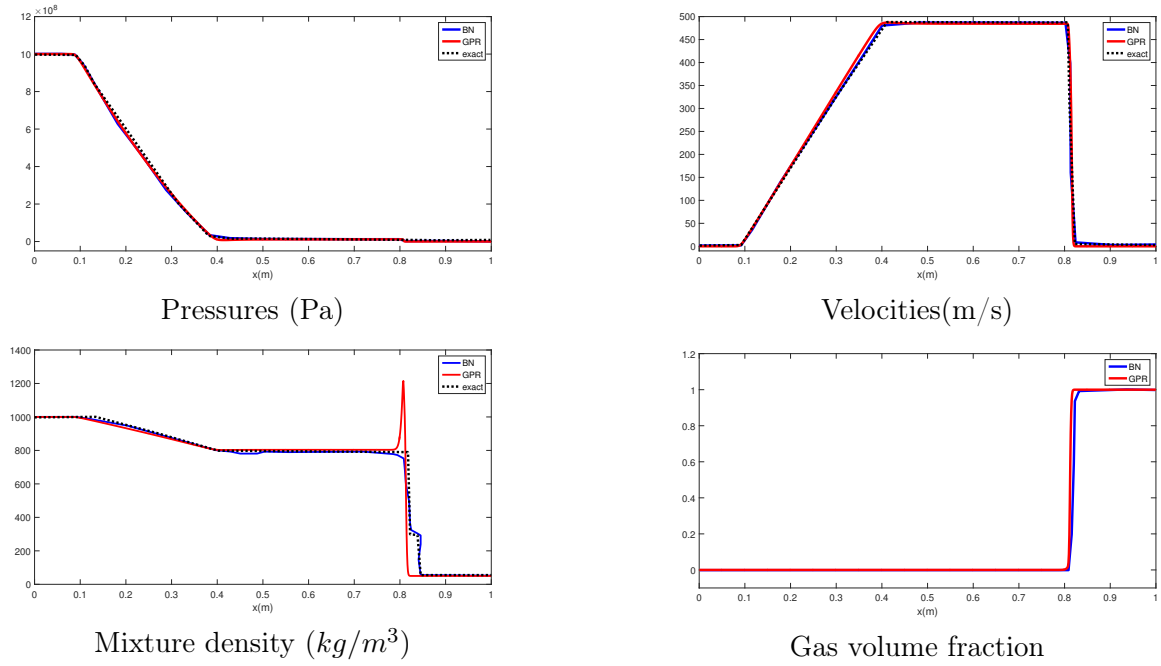
A high-order MUSCL-Hancock finite volume scheme in conjunction with path-conservative is employed.

Graphics of phases pressure, phases velocity, volume fraction and mixture density for the time moment $229\mu s$ are shown in the figure 1. The curves in red correspond to a GPR approach, blue lines correspond to BN model. A black dotted line displays an exact solution.

The graphs of pressures, velocities and densities show in fact five curves: red curve, corresponding to GPR model actually consists of two superposed curves (one for liquid and one for gas component), and blue curve as well consists of two curves of different components. The fifth curve (in black) is a single exact solution. In both GPR and BN cases these numerical curves for different phases are indiscernible. And that tell us a distinctive result of the pressure and velocity relaxation procedures, which give an accurate relaxed state. The phase volume fraction obtained via GPR model is compared with BN model and is not compared with the exact solution because no exact solution exists for the variables.

One can see a good agreement between the results for phase pressures and velocities and their congruence with an exact solution. On the graphic of gas volume fraction we can note a slight difference of the perturbation propagation speed for GPR and BN model. A bit higher value of that speed for BN model than for GPR. That is due to the fact that finite wave speeds are included in GPR model by the definition of the last and their value are not affected by the numerical scheme effects, that in general cases is calculated taking into account different current variables meaning.

An interesting scheme effect can be seen at the mixture density plot. A red (GPR) curve makes quite strong jump at the contact break up zone. This may make one conclude that a bug in a scheme takes place. However it becomes clear if we have a look at the density definition in GPR model,in system 2. The total density is calculated as a sum of weighted densities of its components ($\rho_{total} = \sum \alpha_i \rho_i$, where index i refers to a distinct component). Due to the fact that at the moment of rupture both volume concentrations are nonzero (according to the model definition with the distortion tensor presenting in all the domain), the density of the system takes on a value higher than elsewhere in the flow, therefore, a jump occurs. Nonetheless that effect has no influence on the other parameters of the flow.



Pressures (Pa) Velocities(m/s)

Mixture density (kg/m^3) Gas volume fraction

Figure 1: Comparison of BN (in blue) and GPR (in red) model. Phase pressure (upper left-side picture), phase velocity (upper right-side picture), mixture density (bottom left-side picture), volume fraction (bottom right-side picture)

Conclusion

A brief but quite complete description of the most budding methods for multiphase modelling, namely BN and GPR, are presented in this paper. The numerical test of the same problem for both methods is demonstrated. Both methods describe the flows via hyperbolic system of equation. The hyperbolicity is a very important property that provides the well-posedeness of the problem. That, in its turn, leads to the opportunity to apply well-developed numerical schemes, their stability, accuracy and other useful features.

BN model employs an additional conservation equation to solve a system closure problem that is regular for general multiphase models. It allows to find a solution for non-conservative terms, deals with the cases of strong shock waves or the flows with non equilibrium effects. This model applies to pure fluids and to mixtures. GPR model takes an idea of applying of a distortion tensor to build a system of governing equations. That makes possible to represent a unified mathematical model for both fluids and solids mechanics problems. Another distinctive point of that model is its suitability for the use of advanced high-accuracy Godunov-type numerical methods. It gives an accurate solution for the main characteristics of multiphase problem.

With the help of the demonstrated numerical test we can observe a good agreement of the GPR results with the ones of BN model, that reassures in its applicability and efficiency. For some non-conservative terms, as a volume fraction for example, GPR gives even more correct distribution and shear sound speed. Taking into account an accuracy of GPR model and its great area of application not just for fluids but for both liquid and solid media, authors

consider a new GPR approach a very promising approach and efficient tool for industrial and scientific tasks.

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References

[1] M. Baer and J. Nunziato. A two-phase mixture theory for the deflagration-to-detonation transition in reactive granular materials. *Journal of Multiphase Flows*, 12(6), 1986.

[2] S. Godunov and E. Romenskii. Nonstationary equations of nonlinear elasticity theory in eulerian coordinates. *Journal of Applied Mechanics and Technical Physics*, 1972.

[3] I. Peshkov and E. Romenski. A hyperbolic model for viscous newtonian flows. *Journal of Continuum Mechanics and Thermodynamics*, 28:85–104, 2016.

[4] I . Peshkov, E. Romenski, and M. Dumbser. A unified hyperbolic formulation for viscous fluids and elastoplastic solids. 2017.

[5] S. Godunov and E. Romenskii. *Elements of mechanics of continuous media and conservation laws*. Nauchnaya kniga, Novosibirsk (in Russian).

[6] V. Titarev and E. Toro. Ader: Arbitrary high order godunov approach. *Journal of Scientific Computing*, 17, 2002.

[7] M.Dumbser, I. Peshkov, E. Romenski, and O. Zanotti. High order ader schemes for a unified first order hyperbolic formulation of newtonian continuum mechanics coupled with electro-dynamics. *Journal of Computational Physics*, 358:298–342, 2017.

[8] L. Segel D. Drew. Averaged equations for two-phase flows. *Studies in Applied Mathematics*, 1, 1971.

[9] C. Truesdell. *Rational Thermodynamics*. McGraw-Hill, New York, 1984.

[10] E. Romensky E. Toro, A. Resnyansky. Conservative hyperbolic formulation for compressible two-phase flow with different phase pressures and temperatures. *Quarterly of applied mathematics*, LXV, 2007.

[11] A. Lyapin V. Ryzhov K. Trachenko V. Brazhkin, Yu. Fomin. Two liquid states of matter: A dynamic line on a phase diagram. *Physical review*, E85, 2012.

[12] R. Saurel and R. Abgrall. A multiphase godunov method for compressible multifluid and multiphase flows. *Journal of Computational Physics*, 150:425–467, 1999.